Moyal star product approach to the Bohr-Sommerfeld approximation

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Abstract.

The Bohr-Sommerfeld approximation to the eigenvalues of a one-dimensional quantum Hamiltonian is derived through order $\hbar^2$ (i.e., including the first correction term beyond the usual result) by means of the Moyal star product. The Hamiltonian need only have a Weyl transform (or symbol) that is a power series in $\hbar$, starting with $\hbar^0$, with a generic fixed point in phase space. The Hamiltonian is not restricted to the kinetic-plus-potential form. The method involves transforming the Hamiltonian to a normal form, in which it becomes a function of the harmonic oscillator Hamiltonian. Diagrammatic and other techniques with potential applications to other normal form problems are presented for manipulating higher order terms in the Moyal series.

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1. Introduction

In this article we use the Moyal star product to derive the Bohr-Sommerfeld approximation for the eigenvalues of the bound states of a one-dimensional Hamiltonian, including higher order corrections in $\hbar$. We begin by quoting the result,

$$E_n = \left[H(A) + \frac{\hbar^2}{48}\frac{d}{dA}\left(\frac{1}{\omega(A)}\left\langle\{H,H\}_2\right\rangle_\phi\right) + O(\hbar^4)\right]\Bigg|_{A=(n+1/2)\hbar}, \quad (1)$$

which uses the following notation. E_n is the n-th eigenvalue of the quantum Hamiltonian $\hat{H}$, which has Weyl transform (or "symbol") H. The latter is treated as a classical Hamiltonian with action-angle variables (A,ϕ), and is regarded as a function of the action A. The frequency of the classical motion is $\omega(A) = dH/dA$, and the notation $\{H,H\}_2$ refers to the second Moyal bracket, defined in (A.4c) below. This Moyal bracket is otherwise twice the Hessian determinant of the Hamiltonian,

$$\{H,H\}_2 = 2[H_{,xx}H_{,pp} - (H_{,xp})^2)]. \quad (2)$$

The angle brackets $\langle\ldots\rangle_\phi$ represent an average over the angle ϕ. This result is discussed further in subsection 5.1.

This paper assumes some background in the Wigner-Weyl formalism and the Moyal star product. A sampling of references in this area includes Weyl (1927), Wigner (1932), Groenewold (1946), Moyal (1949), Berry (1977), Balazs and Jennings

(1984), Hillery *et al* (1984), Littlejohn (1986), McDonald (1988), Estrada *et al* (1989) and Gracia-Bondía and Várilly (1995).

Our strategy is to use the Wigner-Weyl symbol correspondence and the series representation of the Moyal star product to transform a given Hamiltonian into a function of the harmonic oscillator, at least in a neighborhood in phase space of a fixed point of the classical Hamiltonian. Notable aspects of this calculation are the higher order terms in the Bohr-Sommerfeld formula, the use of the Moyal star product to achieve a normal form transformation, and the development of diagrammatic and other techniques for handling higher order terms in the Moyal series.

In one-dimensional problems with Hamiltonians of the kinetic-plus-potential form, it is straightforward to extend standard WKB methods to higher order in $\hbar$ to find corrections to the usual Bohr-Sommerfeld formula. Results may be found in Bender and Orszag (1978). Several other approaches to the calculation of higher order terms have been proposed in the literature (Maslov and Fedoriuk, 1981; Voros, 1977, 1989; Kurchan *et al* 1989). Our approach is characterized by the use of the Weyl symbol correspondence for the representation of operators, and the Moyal star product for the manipulation of those operators. In a subsequent paper we shall extend our methods to the case of multidimensional, integrable systems (torus quantization).

Recently Colin de Verdière (2004) has presented another approach for calculating higher order corrections to the one-dimensional Bohr-Sommerfeld formula that is based on the Weyl symbol correspondence and the Moyal star product. Colin de Verdière concentrates on the spectrum of the operator, which is manipulated by representing traces of operators as integrals over phase space. In his approach there is no need to examine eigenfunctions. From an algorithmic or computational standpoint, his method is quite simple, the simplest we have seen for calculating higher order terms (certainly simpler than ours). On the other hand, our approach does provide explicit representations of the transformations necessary to construct eigenfunctions. Another difference is that our method can be generalized to the multidimensional case, whereas we could not see how to do that with the method of Colin de Verdière. The generalization of our method was not trivial, however, and it may be that with more effort his could be generalized, too.

The use of the Weyl symbol correspondence for representing operators means that one can handle a wider class of Hamiltonians than the kinetic-plus-potential type (second order differential operators). For example, integral as well as differential operators are allowed. This is important in applications, such as in plasma physics, where such operators arise, and also for the multidimensional generalization where not all the operators of the commuting set need be second order differential operators.

More importantly, the use of the Weyl symbol correspondence means that the calculations take place in phase space, not configuration space. For example, there is no trouble with caustics or turning points. (Phase space methods are not necessarily free of caustic difficulties, but caustics make no appearance in our approach.) For another example, the usual (lowest order) Bohr-Sommerfeld formula has an obvious invariance under arbitrary canonical transformations, since the energy eigenvalues are expressed in terms of the area of the classical orbits in phase space. To make this statement precise, however, one would have to say precisely what the classical Hamiltonian corresponding to a given quantum Hamiltonian is, over a wider class of operators than those of the kinetic-plus-potential type (a form that is not invariant under canonical transformations). The Weyl symbol correspondence does this, and provides a formalism that is covariant under

linear canonical transformations. Thus, in approaches based on the Weyl symbol correspondence, the lowest order Bohr-Sommerfeld energy eigenvalues are invariant under aribitrary canonical transformations, and the next and all higher order terms in the $\hbar$ series are invariant under linear canonical transformations.

The basic idea of this paper arises from the usual, lowest order Bohr-Sommerfeld formula, which states that the eigenvalues of a quantum Hamiltonian are given approximately by setting $A = (n + 1/2)\hbar$ in the classical formula expressing the classical Hamiltonian H as a function of its action A, $H = f(A)$. This formula suggests that the quantum Hamiltonian is a function of a quantum "action operator," of which the classical formula is a lowest order representation by means of symbols, and that the eigenvalues of the action operator are $(n+1/2)\hbar$. Since these are also the eigenvalues of the harmonic oscillator (of unit frequency), the suggestion is that the action operator is unitarily equivalent to the harmonic oscillator Hamiltonian. If this is so, then the quantum Hamiltonian is unitarily equivalent to a function of the harmonic oscillator. In this paper we find that these suggestions are borne out, and we are able to construct explicitly the unitary operator (or at least the symbol of its generator), in the sense of a formal series in $\hbar$, which transforms a given quantum Hamiltonian into a function of the harmonic oscillator. We only require that the quantum Hamiltonian have a "slowly varying" (defined below) Weyl symbol, and that the symbol have a generic extremum (fixed point) at some point in phase space. The classical analog of the unitary transformation we construct is a canonical transformation that maps the level sets of the classical Hamiltonian around the extremum (which are topological circles) into exact circles about the origin. The latter, of course, are the level sets of the harmonic oscillator.

The transformed Hamiltonian can be regarded as a normal form, that is, a standard or especially simple form achieved by means of a transformation. In this case, the normal form is a function of the harmonic oscillator, achieved on the level of $\hbar$-series for the Weyl symbol and brought about by unitary transformations. The class of Hamiltonians which can be brought into this normal form are those whose symbol has certain properties, notably that of having a family of level sets of circular topology surrounding a generic fixed point. This is the most generic case for bound states in a one-dimensional system, and therefore the one to examine first. But one can imagine that there are other normal forms that apply in other cases, for example, if the fixed point is not generic perhaps a standard quartic oscillator is a normal form. Or if in a certain region of phase space the symbol has a separatrix surrounding two islands of equal area and crossing in one unstable fixed point, perhaps a standard, symmetric double well oscillator is a normal form. Certainly at lowest order in $\hbar$ the unitary transformation is represented by a canonical transformation that preserves area in phase space, so the separatrix of the Hamiltonian and that of the normal form must enclose the same area if they are to be unitarily equivalent. Whether this is enough to guarantee the equivalence of the operators (that is, the equality of their symbols to all orders in $\hbar$) is an open question, as far as we know.

Normal form transformations of operators or sets of operators, either by star product methods or by Fourier integral operators, have been around for some time, in fact we ourselves have used the star product to diagonalize or block diagonalize systems of coupled wave equations (Littlejohn and Flynn, 1991) and to study problems of mode conversion (Littlejohn and Flynn, 1992, 1993). Such methods are well suited to the development of systematic perturbation methods for quantum adiabatic systems, such as molecules in the Born-Oppenheimer approximation (Littlejohn and Weigert,

1993). Similar normal form transformations for coupled wave equations have also been discussed by Braam and Duistermaat (1995), although with the idea of using Fourier integral operators to carry out the transformations instead of star products. The star product approach to normal form transformations for coupled wave equations (WKB on vector bundles) was put on firmer mathematical foundations and generalized in various ways by Emmrich and Weinstein (1996) and Emmrich and Römer (1998). More recently, Colin de Verdière *et al* (1999) have studied normal forms for mode conversion (generalized Landau-Zener transitions) and Colin de Verdiére and Parisse (1999) have studied them for problems involving separatrices. We also expect normal form theory to have applications in transition state theory (Creagh, 2004).

In recent years there has arisen the subject of deformation quantization, which involves generalizations of the Moyal star product to nontrivial phase spaces (symplectic or Poisson manifolds). The phase space $\mathbb{R}^2$ used in this paper, upon which the Weyl symbol correspondence is based, is considered trivial. The general idea is to deform the commutative algebra of multiplication of functions on the phase space into a noncommutative but associative algebra, where $\hbar$ is the deformation parameter and where the new multiplication rule is the generalized star product. It is also required that the order $\hbar$ term in the symbol representation of the commutator be proportional to the Poisson bracket. The new algebra is then interpreted as an algebra of operators on a quantum system, the "quantized" version of the classical phase space. In one approach, the star product is represented as a formal power series in $\hbar$, a generalization of the Moyal formula, and one must work out the terms of the series subject to the constraint of associativity and the appearance of the Poisson bracket at first order. Basic references in this area include Bayen *et al* (1978), Fedosov (1994) and Kontsevich (2003). These works show an interesting geometrical structure associated with the higher order terms in the Moyal star product, which has stimulated our interest in higher order terms in the Bohr-Sommerfeld formula. Our results may be relevant for attempts to understand eigenfunctions of an operator geometrically as noncommutative versions of tori.

It should be possible to read the main body of this paper, skipping the appendices, to obtain an overview of our calculation. The appendices, however, are needed for the details, including notational conventions.

2. The setup

Let $\hat{H}$ be a Hermitian operator (the "Hamiltonian") in a one-dimensional quantum system, that is, $\hat{H}$ acts on wave functions $\psi(x)$, $x \in \mathbb{R}$ (the Hilbert space is $L^2(\mathbb{R})$). We uniformly use hats ($\hat{}$) over a letter to denote operators, whereas a letter without a hat represents the Weyl transform (or Weyl "symbol") of the operator. For example,

$$H(x,p) = \int ds\, e^{-ips/\hbar} \langle x + s/2|\hat{H}|x - s/2\rangle \tag{3}$$

and

$$\hat{H} = \int \frac{dx\, dx'\, dp}{2\pi\hbar} e^{ip(x'-x)/\hbar} H\left(\frac{x+x'}{2}, p\right) |x\rangle\langle x'| \tag{4}$$

illustrate the Weyl transform and its inverse in the case of the Hamiltonian. We regard H as the "classical Hamiltonian," defined on the phase space $\mathbb{R}^2$, with coordinates (x,p). We denote these coordinates collectively by $z^\mu = (x,p)$, $\mu = 1,2$.

We assume that the symbol H has an expansion in $\hbar$ beginning with the power $\hbar^0$,

$$H = H_0 + \hbar H_1 + \hbar^2 H_2 + \dots, \tag{5}$$

where each H_n is independent of $\hbar$. An operator whose symbol possesses this type of expansion will be called "slowly varying". Not all operators are slowly varying; for example, the unitary operator $\exp(-i\hat{H}t/\hbar)$ is not. The leading term (H_0 in the example above) of the symbol of a slowly varying operator will be called the "principal symbol."

We assume H is smooth and has a generic extremum (a fixed point) at some point of phase space. The fixed point need not be at $p = 0$, nor does H need to be invariant under time-reversal ($p \to -p$). An extremum is considered generic if the Hessian matrix $H_{,\mu\nu}$ of the Hamiltonian is nonsingular at the extremum. Here and below we use comma notation for derivatives, for example,

$$H_{,\mu\nu} = \frac{\partial^2 H}{\partial z^\mu \partial z^\nu}. \tag{6}$$

For example, the fixed point $(x, p) = (0, 0)$ of the quartic oscillator ($V(x) = x^4$) is not generic, because the Hessian matrix has rank 1 at the fixed point.

It is convenient in what follows to assume that the extremum is a minimum (always the case for kinetic-plus-potential Hamiltonians). If not, we replace $\hat{H}$ by $-\hat{H}$ at the beginning of the calculation.

Radial equations (on which x is the radial variable $r \geq 0$) are excluded from our formalism, because the Weyl symbol correspondence is not defined in the usual way on the half line, and because the centrifugal potential is singular. We believe the best way to handle such problems within a formalism like the one presented in this paper is by reduction from a problem on a higher dimensional configuration space $\mathbb{R}^n$ under some symmetry, typically $SO(n)$. Nor are singular potentials such as the Coulomb potential covered by this formalism, because singularities generally invalidate the Moyal star product expansion in $\hbar$, itself an asymptotic expansion. The usual lowest order Bohr-Sommerfeld formula usually does give correct answers for singular potentials, at least to leading order in $\hbar$, but the structure of the higher order terms (which powers of $\hbar$ occur, whether the corrections can be represented by powers of $\hbar$ at all, etc.) presumably depend on the nature of the singularity.

In view of our assumptions, the classical Hamiltonian H has level sets in some neighborhood of the fixed point that are topological circles. We concentrate on this region of phase space, and ignore any separatrices and changes in the topology of the level sets of H which may be encountered further away from the fixed point.

For convenience we perform a canonical scaling on the coordinates (x, p) (or operators $(\hat{x}, \hat{p})$) to cause them both to have units of action$^{1/2}$. For example, in the case of the ordinary harmonic oscillator, we would write $x' = \sqrt{m\omega}\, x$, $p' = p/\sqrt{m\omega}$, and then drop the primes.

The strategy will be to perform a sequence of unitary operations that transform the original Hamiltonian $\hat{H}$ into a new Hamiltonian that is a function of the harmonic oscillator Hamiltonian, at least in the "microlocal" sense of the symbols in the neighborhood of the fixed point. Since unitary transformations do not change the spectrum of an operator, the new Hamiltonian will have the same spectrum as the old one. But since the new Hamiltonian is a function of the harmonic oscillator Hamiltonian, its eigenvalues are easy to compute.

The transformations will proceed in two stages. In the first stage, we perform a "preparatory" transformation that maps $\hat{H}$ into a new Hamiltonian $\hat{K}$ that is a function of the harmonic oscillator Hamiltonian at lowest order in $\hbar$. We follow this by a sequence of near-identity unitary transformations that transform $\hat{K}$ into a new Hamiltonian $\hat{M}$ that is a function of the harmonic oscillator Hamiltonian to all higher orders in $\hbar$, at least formally. Thus, the stages are

$$\hat{H} \to \hat{K} \to \hat{M}. \tag{7}$$

What we mean by the harmonic oscillator Hamiltonian is really the action of the harmonic oscillator, given in operator and symbol form by

$$\hat{I} = \frac{1}{2}(\hat{x}^2 + \hat{p}^2), \qquad I = \frac{1}{2}(x^2 + p^2). \tag{8}$$

It turns out that an operator is a function $\hat{I}$ if and only if its symbol is a function of I, as will be discussed more fully below, although the two functions are not the same beyond lowest order in $\hbar$. Thus, to ensure that the transformed Hamiltonian is a function of $\hat{I}$, we require that its symbol be a function of I.

3. The preparatory transformation

The preparatory transformation (the first arrow in (7)) is the most difficult, because it is not a near-identity transformation and cannot be handled by Lie algebraic (power series) methods. This transformation will transform $\hat{H}$ into another Hamiltonian $\hat{K}$ whose symbol is a function of I plus terms of order $\hbar^2$ and higher. Thus, the principal symbol of $\hat{K}$ will be a function of I. The preparatory transformation only makes the leading order term in the symbol of $\hat{K}$ a function of I, not the higher order terms.

3.1. Imbedding $\hat{H}$ and $\hat{U}$ in a family

Let $\hat{H}$ be given. Ultimately, we shall seek a unitary transformation $\hat{U}$ such that the new Hamiltonian $\hat{K}$, defined by

$$\hat{K} = \hat{U}\hat{H}\hat{U}^\dagger, \qquad \hat{H} = \hat{U}^\dagger\hat{K}\hat{U}, \tag{9}$$

has a symbol K that is a function of I plus terms of order $\hbar^2$ and higher.

For the moment, however, it is conceptually simpler to imagine that $\hat{H}$ and $\hat{U}$ are given, and to seek a means based on Weyl symbols of computing $\hat{K}$, without regard to the functional form of K. We do this by imbedding $\hat{U}$ in a family, $0 \le \epsilon \le 1$, that is by assuming that there exists a smooth family of unitary operators $\hat{U}_\epsilon$, such that

$$\hat{U}_\epsilon = \begin{cases} 1 & \text{if } \epsilon = 0, \\ \hat{U} & \text{if } \epsilon = 1. \end{cases} \tag{10}$$

The family $\hat{U}_\epsilon$ can be seen as a path in the group of unitary transformations that act on Hilbert space, connecting the identity and the final $\hat{U}$. We do not assume ϵ is small, and we do not carry out any power series expansion in ϵ. We imbed $\hat{H}$ in a similar family, defining

$$\hat{H}_\epsilon = \hat{U}_\epsilon^\dagger\, \hat{K}\, \hat{U}_\epsilon, \tag{11}$$

so that

$$\hat{H}_\epsilon = \begin{cases} \hat{K} & \text{if } \epsilon = 0, \\ \hat{H} & \text{if } \epsilon = 1. \end{cases} \tag{12}$$

Table 1. Notation for operators, symbols and functions depending on ϵ.

$\epsilon = 0$	1	K	K_n	Id^μ	θ	I
any ϵ	U_ϵ	H_ϵ	$H_{n\epsilon}$	Z^μ_ϵ	ϕ_ϵ	A_ϵ
$\epsilon = 1$	U	H	$\delta_{n0}\, H$	Z^μ	ϕ	A

One might say that the ϵ-evolution runs backwards, since $\hat{K}$ evolves into $\hat{H}$ as ϵ goes from 0 to 1. As always, Weyl symbols of the operators above are denoted without the hat, for example, U, K, U_ϵ, H_ϵ. There are several operators, symbols and functions in this paper that depend on ϵ, the notation for which is summarized in Table 1. We shall be interested in calculating $\hat{H}_\epsilon$, from which $\hat{K}$ follows by setting $\epsilon = 0$.

We obtain a differential equation for $\hat{H}_\epsilon$ by differentiating (11), which gives

$$\frac{d\hat{H}_\epsilon}{d\epsilon} = \frac{i}{\hbar}[\hat{G}_\epsilon, \hat{H}_\epsilon], \tag{13}$$

where the Hermitian operator $\hat{G}_\epsilon$ (the "generator") is defined by

$$\hat{G}_\epsilon = i\hbar\, \hat{U}^\dagger_\epsilon \frac{d\hat{U}_\epsilon}{d\epsilon} = -i\hbar \frac{d\hat{U}^\dagger_\epsilon}{d\epsilon}\, \hat{U}_\epsilon = \hat{G}^\dagger_\epsilon. \tag{14}$$

We assume that $\hat{G}_\epsilon$ is slowly varying. We shall solve (13) by converting operators to symbols and using the Moyal product formula. See Appendix A for the Moyal star product and the diagrammatic notation we shall use for the functions and operations that arise from it.

3.2. Differential equations for H_ϵ and $H_{n\epsilon}$

We now transcribe (13) to symbols and substitute (A.6). This gives a differential equation for the symbol H_ϵ,

$$\frac{dH_\epsilon}{d\epsilon} = -\{G_\epsilon, H_\epsilon\} + \frac{\hbar^2}{24}\{G_\epsilon, H_\epsilon\}_3 - \frac{\hbar^4}{1920}\{G_\epsilon, H_\epsilon\}_5 + \ldots, \tag{15}$$

which is subject to the boundary condition $H_\epsilon = H$ at $\epsilon = 1$. We express the solution of this equation in terms of a set of new functions or symbols, $H_{0\epsilon}$, $H_{2\epsilon}$, etc., which are required to satisfy the differential equations,

$$\frac{dH_{0\epsilon}}{d\epsilon} - \{H_{0\epsilon}, G_\epsilon\} = 0, \tag{16a}$$

$$\frac{dH_{2\epsilon}}{d\epsilon} - \{H_{2\epsilon}, G_\epsilon\} = \frac{1}{24}\{G_\epsilon, H_{0\epsilon}\}_3, \tag{16b}$$

$$\frac{dH_{4\epsilon}}{d\epsilon} - \{H_{4\epsilon}, G_\epsilon\} = \frac{1}{24}\{G_\epsilon, H_{2\epsilon}\}_3 - \frac{1}{1920}\{G_\epsilon, H_{0\epsilon}\}_5, \tag{16c}$$

etc., and the boundary condition $H_{n\epsilon} = \delta_{n0}\, H$ at $\epsilon = 1$. Then we have

$$H_\epsilon = H_{0\epsilon} + \hbar^2 H_{2\epsilon} + \hbar^4 H_{4\epsilon} + \ldots. \tag{17}$$

This is not an expansion of H_ϵ in powers of $\hbar$ as in (5), because the functions $H_{n\epsilon}$ are themselves allowed to have a dependence on $\hbar$. But each of these is slowly varying, so that if the series (17) is truncated, the order of the omitted term is given by the $\hbar$ coefficient. Finally, we define $K_n = H_{n\epsilon}$ evaluated at $\epsilon = 0$ (see Table 1), so that we have an expansion of the symbol K of $\hat{K}$,

$$K = K_0 + \hbar^2 K_2 + \hbar^4 K_4 + \ldots. \tag{18}$$

The solutions of (16a)–(16c) can be expressed in terms of a certain ϵ-dependent, classical canonical transformation, $z'^{\mu}(\epsilon) = Z^{\mu}_{\epsilon}(z)$, where z and z' are the old and new variables, and Z^{μ}_{ϵ} is the transformation function. The family of canonical transformations Z^{μ}_{ϵ} reduces to the identity at $\epsilon = 0$, while at $\epsilon = 1$ we shall denote the transformation simply by Z^{μ} (without the ϵ). See Table 1. The transformation Z^{μ}_{ϵ} will be defined momentarily, but it turns out that the left hand sides of (16a)–(16c) are convective derivatives along the associated Hamiltonian flow. Equation (16a) is a homogeneous equation for the unknown $H_{0\epsilon}$, and the others are inhomogeneous equations with driving terms determined by lower order solutions. The structure of the system is that of a Dyson expansion, in which the canonical transformation Z^{μ}_{ϵ} specifies a kind of interaction representation. The definition of Z^{μ}_{ϵ} requires some notational understandings that are presented in Appendix B.

3.3. The canonical transformations Z and Z_ϵ

The canonical transformation Z^{μ}_{ϵ} is defined as the solution of the functional differential equation,

$$\frac{dZ^{\mu}_{\epsilon}}{d\epsilon} = \{Z^{\mu}_{\epsilon}, G_{\epsilon}\}, \tag{19}$$

subject to the initial conditions, $Z^{\mu}_{\epsilon} = \mathrm{Id}^{\mu}$ at $\epsilon = 0$, and we define $Z^{\mu} = Z^{\mu}_{\epsilon}$ at $\epsilon = 1$ (see Table 1). The functions Z^{μ}_{ϵ} so defined constitute a canonical transformation, for if we compute the ϵ-derivative of their Poisson brackets among themselves, we find

$$\frac{d}{d\epsilon}\{Z^{\mu}_{\epsilon}, Z^{\nu}_{\epsilon}\} = \{\{Z^{\mu}_{\epsilon}, G_{\epsilon}\}, Z^{\nu}_{\epsilon}\}+\{Z^{\mu}_{\epsilon}, \{Z^{\nu}_{\epsilon}, G_{\epsilon}\}\} = -\{G_{\epsilon}, \{Z^{\mu}_{\epsilon}, Z^{\nu}_{\epsilon}\}\}, \tag{20}$$

where we have used the Jacobi identity. These are subject to the initial conditions $\{Z^{\mu}_{\epsilon}, Z^{\nu}_{\epsilon}\} = J^{\mu\nu}$ at $\epsilon = 0$. But since $J^{\mu\nu} = \mathrm{const}$, the initial conditions are the solution for all ϵ, as shown by direct substitution.

The canonical transformation Z^{μ}_{ϵ} is not generated by G_{ϵ} regarded as an ϵ-dependent Hamiltonian function, but rather by $G'_{\epsilon} = G_{\epsilon} \circ Z^{-1}_{\epsilon}$. That is, if we write $z^{\mu}(\epsilon) = Z^{\mu}_{\epsilon}(z_0)$ for the solution of Hamilton's equations,

$$\frac{dz^{\mu}}{d\epsilon} = J^{\mu\nu}\, G'_{\epsilon,\nu}(z), \tag{21}$$

then the functions Z^{μ}_{ϵ} satisfy

$$\frac{dZ^{\mu}_{\epsilon}}{d\epsilon} = J^{\mu\nu}\, G'_{\epsilon,\nu} \circ Z_{\epsilon} = \{\mathrm{Id}^{\mu}, G'_{\epsilon}\} \circ Z_{\epsilon} = \{Z^{\mu}_{\epsilon}, G_{\epsilon}\}, \tag{22}$$

which agrees with (19). In the final step we have used an important property of the Poisson bracket, namely, that if A and B are any two functions and Z is a canonical transformation (symplectic map), then

$$\{A, B\} \circ Z = \{A \circ Z, B \circ Z\}. \tag{23}$$

3.4. Notation for ϵ-derivatives

The following notation will be useful for carrying out differentiations and integrations in the interaction representation, specified by composing a function with Z^{-1}_{ϵ}.

For any function F_{ϵ} on phase space, possibly ϵ-dependent, we define

$$\frac{DF_{\epsilon}}{D\epsilon} = \left[\frac{d}{d\epsilon}(F_{\epsilon} \circ Z^{-1}_{\epsilon})\right] \circ Z_{\epsilon}, \tag{24}$$

for a kind of derivative operator in the interaction representation. This can be written in an alternative form,

$$\frac{DF_\epsilon}{D\epsilon} = \frac{dF_\epsilon}{d\epsilon} - \{F_\epsilon, G_\epsilon\}. \tag{25}$$

The proof of (25) is obtained by setting $F'_\epsilon = F_\epsilon \circ Z_\epsilon^{-1}$, so that

$$\frac{dF_\epsilon}{d\epsilon} = \frac{d}{d\epsilon}(F'_\epsilon \circ Z_\epsilon) = \frac{dF'_\epsilon}{d\epsilon} \circ Z_\epsilon + (F'_{\epsilon,\mu} \circ Z_\epsilon)\frac{dZ^\mu_\epsilon}{d\epsilon}. \tag{26}$$

But by (19) and the chain rule for the Poisson bracket, the final term can be written,

$$(F'_{\epsilon,\mu} \circ Z_\epsilon)\{Z^\mu_\epsilon, G_\epsilon\} = \{F'_\epsilon \circ Z_\epsilon, G_\epsilon\} = \{F_\epsilon, G_\epsilon\}. \tag{27}$$

Rearranging the result gives (25).

3.5. Solutions for $H_{n\epsilon}$ and K_n

In view of (25), the left hand sides of (16*a*)–(16*c*) can now be written $DH_{n\epsilon}/D\epsilon$. In particular, (16*a*) is simply $DH_{0\epsilon}/D\epsilon = 0$, which immediately gives $H_{0\epsilon} = C \circ Z_\epsilon$, where C is a function independent of ϵ. Substituting $\epsilon = 1$ and the boundary condition shown in Table 1, we find $H = C \circ Z$. Then substituting $\epsilon = 0$, we find $C = K_0$. In summary,

$$H_{0\epsilon} = K_0 \circ Z_\epsilon. \tag{28}$$

In particular, substituting $\epsilon = 1$ we obtain

$$H = K_0 \circ Z, \qquad K_0 = H \circ Z^{-1}. \tag{29}$$

This completes the solution of H_ϵ and K to lowest order.

The second order equation (16*b*) can now be written

$$\frac{DH_{2\epsilon}}{D\epsilon} = \frac{1}{24}\{G_\epsilon, H_{0\epsilon}\}_3. \tag{30}$$

We use (24) in this, compose both sides with Z_ϵ^{-1}, integrate between ϵ and 1, and use the boundary condition $H_{2\epsilon} = 0$ at $\epsilon = 1$. The result is

$$H_{2\epsilon} = -\frac{1}{24}\int_\epsilon^1 d\epsilon' \, \{G_{\epsilon'}, H_{0\epsilon'}\}_3 \circ Z_{\epsilon'}^{-1} \circ Z_\epsilon. \tag{31}$$

Finally, setting $\epsilon = 0$, we have

$$K_2 = -\frac{1}{24}\int_0^1 d\epsilon \, \{G_\epsilon, H_{0\epsilon}\}_3 \circ Z_\epsilon^{-1}. \tag{32}$$

Similarly, we solve the fourth order equation (16*c*), finding

$$K_4 = -\frac{1}{24}\int_0^1 d\epsilon \, \{G_\epsilon, H_{2\epsilon}\}_3 \circ Z_\epsilon^{-1} + \frac{1}{1920}\int_0^1 d\epsilon \, \{G_\epsilon, H_{0\epsilon}\}_5 \circ Z_\epsilon^{-1}. \tag{33}$$

Clearly the solutions for $H_{n\epsilon}$ and K_n at any order n can be written in terms of integrals over lower order solutions.

Let us now choose $\hat{U}$ so that K will be a function of I at lowest order in $\hbar$. We shall work backwards, first finding a canonical transformation Z such that $K_0 = H \circ Z^{-1}$ is a function of I. We then imbed this in a one parameter family Z_ϵ, from which we compute G_ϵ, $\hat{G}_\epsilon$, $\hat{U}_\epsilon$, and finally $\hat{U}$.

3.6. Construction of Z via action-angle variables

The desired canonical transformation Z can be specified in terms of the action-angle variables for the original Hamiltonian H and the harmonic oscillator. We let (A, ϕ) be the action-angle variables of H, according to the standard construction in classical mechanics, although we note that H may depend on $\hbar$. The action is defined as a function of the energy by

$$A(E) = \frac{1}{2\pi} \int_{H<E} dp\, dx. \tag{34}$$

The integral is taken over the interior of the closed curve $H = E$ (a level set of H). The action vanishes at the fixed point, and is an increasing function of energy as we move away from it. Equation (34) is the standard way to write the definition of the action, but, keeping in mind the warnings of Appendix B, if we wish to think of A as a function on phase space, that is, a mapping : $\mathbb{R}^2 \to \mathbb{R}$ then it makes no sense to write $A(E)$. When we say that the action and energy are functions of one another, what we mean is

$$H = f_0 \circ A, \tag{35}$$

where $f_0 : \mathbb{R} \to \mathbb{R}$ is the function of a single variable expressing the relationship between energy and action. (The 0 subscript will be explained below.) The function f_0 is invertible in the region of interest, so $A = f_0^{-1} \circ H$. Then (34) can be written more properly by picking a point z in the region in question, writing $E = H(z)$, and then writing

$$A(z) = (f_0^{-1} \circ H)(z) = f_0^{-1}(E), \tag{36}$$

instead of the left hand side of (34). Having defined the action A, we then define the conjugate angle ϕ by standard means in classical mechanics (through a generating function). This involves a choice of origin (a point where $\phi = 0$) on each of the closed curves $H = E$ in the region of phase space under consideration. This choice is smooth but arbitrary. We henceforth regard A and ϕ as specific functions : $\mathbb{R}^2 \to \mathbb{R}$.

Next we introduce the harmonic oscillator action-angle variables (I, θ), where I is given by (8) and θ is the conjugate angle (the geometrical polar angle in the phase plane, increasing in the clockwise direction). These are regarded as functions : $\mathbb{R}^2 \to \mathbb{R}$. Then the canonical transformation $Z : \mathbb{R}^2 \to \mathbb{R}^2$ is defined by

$$\begin{aligned} A &= I \circ Z, \\ \phi &= \theta \circ Z, \end{aligned} \tag{37}$$

which uniquely defines Z, since (A, ϕ), $z = (x, p)$, and (I, θ) are invertible functions of each other (in the regions of interest). Then, using the definition (29) of K_0, we have

$$K_0 = H \circ Z^{-1} = f_0 \circ A \circ Z^{-1} = f_0 \circ I, \tag{38}$$

that is, K_0 is the same function of the harmonic oscillator action I as H is of its own action A. This is reasonable, since canonical transformations preserve area, and the action is proportional to the area inside a level set. In particular, with this choice of Z, the level sets of K_0 are circles.

The smoothness of Z is relevant for the use of the Moyal star product series (A.1) which involves derivatives of functions on phase space. We believe that Z is smooth at all points of the relevant domain, under the assumption that H is smooth and has a generic fixed point. If the fixed point is not generic (for example, the quartic oscillator), then Z need not be smooth. These questions are discussed further in Appendix C.

3.7. Finding Z_ϵ, G_ϵ and $\hat{U}_\epsilon$

Now that we have Z, we imbed it in a smooth family Z_ϵ with the boundary values shown in Table 1. Sjöstrand and Zworski (2002) show that this can be done in a neighborhood of the fixed point, and Evans and Zworski (2004) give another proof that applies in the full domain. For later reference, we also define ϵ-dependent versions of the action-angle variables,

$$A_\epsilon = I \circ Z_\epsilon, \tag{39a}$$

$$\phi_\epsilon = \theta \circ Z_\epsilon, \tag{39b}$$

with boundary values shown in Table 1. Then we have

$$H_{0\epsilon} = f_0 \circ A_\epsilon. \tag{40}$$

All three Hamiltonians, H, $H_{0\epsilon}$ and K are the same function (f_0) of their own actions (A, A_ϵ and I, respectively).

Next we wish to find a function G_ϵ such that (19) is satisfied for the given Z_ϵ. This can always be done, since that equation can be solved for the derivatives $G_{\epsilon,\mu}$, the components of a closed 1-form (hence exact, since the region is contractible). This is a standard result in classical mechanics (Arnold, 1989), which is summarized in component language in Appendix E. The function G_ϵ is determined to within an ϵ-dependent, additive constant. In the following we drop this constant, since its only effect is to introduce an ϵ-dependent phase into $\hat{U}_\epsilon$, which has no effect on the transformed Hamiltonian.

Finally, given G_ϵ, we transform it into the operator $\hat{G}_\epsilon$, and then define $\hat{U}_\epsilon$ as the solution of

$$\frac{d\hat{U}_\epsilon}{d\epsilon} = -\frac{i}{\hbar}\hat{U}_\epsilon \hat{G}_\epsilon, \tag{41}$$

subject to the initial condition $\hat{U}_\epsilon = 1$ at $\epsilon = 0$. Then we set $\hat{U} = \hat{U}_\epsilon$ at $\epsilon = 1$. This completes the preparatory transformation (the construction of $\hat{U}$ such that $\hat{K}$ has a symbol that is a function of I at lowest order). We do not need to solve (41) explicitly, since for the purposes of this paper we only need to calculate the effect on the symbol of a slowly varying operator when it is conjugated by $\hat{U}$. But it is important to know that $\hat{U}$ exists, as we have shown.

The preparatory transformation might have been carried out with oscillatory integrals coming from the integral representation of the Moyal star product, rather than in terms of a path Z_ϵ through the group of canonical transformations. Indeed, we tried this approach initially, but found that it led to complicated algebra beyond lowest order that we were not able to organize to our satisfaction. Perhaps with more effort that approach could be cast into suitable form.

The formalism we have presented is slightly simpler if we assume that the path through the group of canonical transformations, Z_ϵ, $0 \le \epsilon \le 1$, is a one-parameter subgroup, that is, that G_ϵ is independent of ϵ. This, however, is a special assumption that we did not want to make. Moreover, the use of an arbitrary path allows us to study what happens when we vary the path, which leads to interesting conclusions (see below).

4. Second stage transformations

In the second stage (the second arrow in (7)) we transform $\hat{K}$ into a new Hamiltonian $\hat{M}$, such that the symbol M is formally a function of I to all orders in $\hbar$. We do this

by Lie algebraic (power series) techniques that are similar to those used in classical perturbation theory (Dragt and Finn, 1976; Cary 1981), although here there are higher order Moyal brackets appearing as well as Poisson brackets. See also Littlejohn and Weigert (1993) for an example of a Moyal-based perturbation calculation applied to an adiabatic problem in quantum mechanics.

4.1. The higher order transformations

We apply a sequence of near-identity unitary transformations, each of which is responsible for making the symbol of the Hamiltonian a function of I at two successive orders of $\hbar$. Only even powers of $\hbar$ occur in this process. The sequence is defined by

$$\begin{aligned}\hat{M}^{(0)} &= \hat{K},\\ \hat{M}^{(2)} &= \hat{U}_2\,\hat{M}^{(0)}\,\hat{U}_2^\dagger,\\ \hat{M}^{(4)} &= \hat{U}_4\,\hat{M}^{(2)}\,\hat{U}_4^\dagger,\end{aligned} \tag{42}$$

etc., where

$$\hat{U}_n = \exp(-i\hbar^{n-1}\hat{G}_n), \tag{43}$$

and where $\hat{G}_n$ is the n-th order generator, assumed to have a symbol G_n that is slowly varying. Then, for example, the expression for $\hat{M}^{(2)}$ can be written as a series in $\hbar$ involving iterated commutators,

$$\hat{M}^{(2)} = \hat{K} - i\hbar[\hat{G}_2,\hat{K}] - \frac{\hbar^2}{2}[\hat{G}_2,[\hat{G}_2,\hat{K}]] + \ldots, \tag{44}$$

and similarly for $\hat{M}^{(4)}$ etc. Transcribing (44) to symbols and using (A.6), we have

$$M^{(2)} = K + \hbar^2\{G_2,K\} + \hbar^4\left(-\frac{1}{24}\{G_2,K\}_3 + \frac{1}{2}\{G_2,\{G_2,K\}\}\right) + \ldots. \tag{45}$$

In a similar manner we write out commutator expansions for the higher order transformations in (42), transcribe them into symbols, compose the transformations together, and substitute the expansion (18). We write the result in the form,

$$M = M_0 + \hbar^2 M_2 + \hbar^4 M_4 + \ldots, \tag{46}$$

where $M = M^{(\infty)}$, the symbol of the final Hamiltonian after all the second stage unitary transformations have been carried out, and where

$$M_0 = K_0, \tag{47a}$$

$$M_2 = K_2 + \{G_2,K_0\}, \tag{47b}$$

$$M_4 = K_4 + \{G_2,K_2\} - \frac{1}{24}\{G_2,K_0\}_3 + \frac{1}{2}\{G_2,\{G_2,K_0\}\} + \{G_4,K_0\}, \tag{47c}$$

etc. Each M_n is slowly varying.

We want M to be a function only of I. At lowest order we have this already,

$$M_0 = K_0 = f_0 \circ I = H \circ Z^{-1}. \tag{48}$$

At second order, we wish to choose G_2 in (47b) so that M_2 will be a function only of I, that is, independent of θ. In the next few steps it is convenient to bring back the abuse of notation rejected in Appendix B, and to think of functions like K_2, M_2, etc. as functions of either $z = (x,p)$ or of the action-angle coordinates (θ,I),

as convenient. Then the Poisson bracket in (47b) can be computed in action-angle variables, whereupon we have

$$M_2 = K_2 + \frac{\partial G_2}{\partial \theta}\,\omega(I), \tag{49}$$

where $\omega(I) = dK_0/dI$. Note that as a function, $\omega = f_0'$, since $K_0 = f_0 \circ I$, so $\omega(A) = dH/dA = f_0'(A)$. Thus, $\omega(A)$ is the frequency of the classical oscillator with Hamiltonian H. If we now average both sides of (49) over the angle θ, we obtain

$$M_2 = \bar{K}_2, \tag{50}$$

where the overbar represents the θ average. The simple result is that M_2 is just the average of K_2, given by (32).

Then subtracting (50) from (49) and rearranging, we obtain

$$\frac{\partial G_2}{\partial \theta} = -\frac{1}{\omega(I)}\tilde{K}_2, \tag{51}$$

where the tilde represents the oscillatory part in θ of a function. Equation (51) always has a solution G_2 that is a periodic function of θ, that is, it is a single-valued function of (x, p), since $\tilde{K}_2$ has a Fourier series in θ without the constant term. Thus we have shown that it is possible to choose G_2 in (47b) such that M_2 is independent of θ.

The same structure persists at all higher orders. For example, taking the averaged and oscillatory parts of the fourth order equation (47c) yields an expression for M_4 that is independent of θ and a solvable equation for G_4. This shows that it is possible to transform the original Hamiltonian $\hat{H}$ into a function of the harmonic oscillator $\hat{I}$ to all orders in $\hbar$, at least in the sense of a formal power series for the symbol.

4.2. Doing the ϵ-integral

The following steps require some notation and an important theorem regarding averaging operators that are explained in Appendix D. The theorem in question is (D.8), which we apply to (50), using (32), to obtain a useful form of the expression for M_2:

$$\begin{aligned} M_2 &= -\frac{1}{24}\int_0^1 d\epsilon \left\langle \; (G_\epsilon \rightleftarrows H_{0\epsilon}) \; \circ Z_\epsilon^{-1} \right\rangle_\theta \\ &= -\frac{1}{24}\int_0^1 d\epsilon \left\langle \; G_\epsilon \rightleftarrows H_{0\epsilon} \; \right\rangle_{\phi_\epsilon} \circ Z_\epsilon^{-1}, \end{aligned} \tag{52}$$

where the diagrammatic notation is explained in Appendix A. The ϵ-integration in (52) can be done, yielding an expression independent of ϵ, that is, independent of the path taken through the group of unitary or canonical transformations used in the preparatory transformation.

First we transform the integrand of (52) as described in Appendix F, to obtain

$$\begin{aligned} M_2 &= \frac{1}{24}\int_0^1 d\epsilon \left[\frac{d}{dA_\epsilon}\left(\frac{1}{\omega \circ A_\epsilon}\left\langle \; H_{0\epsilon} \rightarrow G_\epsilon \rightleftarrows H_{0\epsilon} \; \right\rangle_{\phi_\epsilon}\right)\right] \circ Z_\epsilon^{-1} \\ &= \frac{1}{24}\frac{d}{dI}\left(\frac{1}{\omega \circ I}\int_0^1 d\epsilon \left\langle \; H_{0\epsilon} \rightarrow G_\epsilon \rightleftarrows H_{0\epsilon} \; \right\rangle_{\phi_\epsilon} \circ Z_\epsilon^{-1}\right) \\ &= \frac{1}{24}\frac{d}{dI}\left(\frac{1}{\omega \circ I}\left\langle \int_0^1 d\epsilon \; (H_{0\epsilon} \rightarrow G_\epsilon \rightleftarrows H_{0\epsilon}) \; \circ Z_\epsilon^{-1} \right\rangle_\theta\right), \end{aligned} \tag{53}$$

where once we have transformed A_ϵ into I by composing with Z_ϵ^{-1} we can pull the factors depending on it out of the integral, since they are no longer ϵ-dependent. Next we use the methods described in Appendix G to guess and prove that

$$\frac{1}{2}\frac{D}{D\epsilon}\left(H_{0\epsilon} \rightleftarrows H_{0\epsilon}\right) \;=\; \left(H_{0\epsilon} \rightarrow G_\epsilon \rightleftarrows H_{0\epsilon}\right) . \tag{54}$$

This makes the integral (53) easy to do, yielding,

$$M_2 = \frac{1}{48}\frac{d}{dI}\left(\frac{1}{\omega\circ I}\left\langle \left(H \rightleftarrows H\right) \circ Z^{-1} - \left(K_0 \rightleftarrows K_0\right) \right\rangle_\theta\right). \tag{55}$$

Let us call the two terms on the right hand side of (55) the "H-term" and the "K_0-term." Since $K_0 = f_0 \circ I$, the Moyal bracket in the K_0-term can be expanded out by the chain rule in terms of derivatives of f_0 and diagrams involving I. We find

$$\left(K_0 \rightleftarrows K_0\right) \;= 2f_0'f_0''\left(I \rightarrow I \leftarrow I\right) \;+ {f_0'}^2\left(I \rightleftarrows I\right) , \tag{56}$$

where f_0' means $f_0'\circ I$, etc., and where some diagrams have vanished since $\left(I \rightarrow I\right) = \{I, I\} = 0$. The nonvanishing diagrams can be calculated using (8), which gives

$$\left(I \rightarrow I \leftarrow I\right) \;= 2I, \qquad \left(I \rightleftarrows I\right) \;= 2, \tag{57}$$

so the K_0-term is a function only of I and the angle average in (55) does nothing to this term. Finally we take the I-derivative and compute the K_0-term explicitly, finding,

$$K_0\text{-term} = -\frac{f_0''}{8} - \frac{f_0'''}{12}I. \tag{58}$$

The intermediate Hamiltonian K is not unique, because of the choice of the path Z_ϵ through the group of canonical transformations that connects the identity at $\epsilon = 0$ and the given transformation Z at $\epsilon = 1$. More precisely, $K_0 = H \circ Z^{-1}$ is unique because it is expressed purely in terms of Z, but K_2 and all higher order terms depend on Z_ϵ at intermediate values of ϵ. Nevertheless, by (50), if we vary the path Z_ϵ while keeping the endpoints fixed, K_2 can change by at most a function whose θ-average is zero, so that M_2 remains invariant. Such a function can be written as the θ-derivative of some other function. These facts are proven in Appendix H.

5. The eigenvalues

We have shown how to transform the original Hamiltonian $\hat{H}$ into a new Hamiltonian $\hat{M}$ whose symbol M is a function of I to any desired order in $\hbar$, and we have explicitly evaluated the first two terms M_0 and M_2 of the series for M. Let us write $M_n = g_n \circ I$, thereby defining the functions g_n, so that $M = g \circ I$, where $g = g_0 + \hbar^2 g_2 + \hbar^4 g_4 + \ldots$. In view of (48) we have $g_0 = f_0$, and g_2 is given implicitly by (55).

As mentioned above, an operator is a function of $\hat{I}$ if and only if its symbol is a function of I. The two functions are the same at lowest order in $\hbar$, but it turns out that they differ at higher order. These facts are proved in Appendix I. Thus, if we define a function f by $\hat{M} = f(\hat{I})$ and expand it according to $f = f_0 + \hbar^2 f_2 + \hbar^4 f_4 + \ldots$, then we will have $f_0 = g_0$ but $f_2 \neq g_2$. Thus f_0 defined this way is the same function introduced above in (35), and we have $\hat{M} = f_0(\hat{I})$ at lowest order. This is just what we guessed in the introduction, and it implies the usual Bohr-Sommerfeld formula, since the eigenvalues of $\hat{I}$ are $(n + 1/2)\hbar$.

5.1. The Bohr-Sommerfeld rule to higher order

To carry the Bohr-Sommerfeld rule to higher order, it is necessary to find the relation between the symbol of an operator and the symbol of a function of that operator. This topic is discussed in Appendix I. In the following we are interested in the case $\hat{M} = f(\hat{I})$ and $M = g \circ I$, so we will identify $\hat{M}$ and $\hat{I}$ with operators $\hat{B}$ and $\hat{A}$ of Appendix I, respectively. Then (I.4) gives the relation between functions f and g. Expanding f and g in even $\hbar$ series as above and using $M_n = g_n \circ I$, we can write (I.4) in the form,

$$\begin{aligned} & M_0 + \hbar^2 M_2 + \dots \\ & = f_0 + \hbar^2 \left[f_2 - \frac{f_0''}{16} \left(I \rightrightarrows I \right) - \frac{f_0'''}{24} \left(I \rightarrow I \leftarrow I \right) \right] + \dots \\ & = f_0 + \hbar^2 \left(f_2 - \frac{f_0''}{8} - \frac{f_0'''}{12} \right) + \dots , \end{aligned} \tag{59}$$

where f_0 means $f_0 \circ I$, etc., and where we use (57). This implies $M_0 = f_0 \circ I$, which we knew already, and allows us to solve for f_2 by equating the final quantity in the parentheses with M_2 in (55). We see that the second order correction terms coming from (I.4) exactly cancel the K_0-term (58), so that $f_2 \circ I$ is just the H-term of (55),

$$f_2 \circ I = \frac{1}{48} \frac{d}{dI} \left(\frac{1}{\omega \circ I} \left\langle \, H \rightrightarrows H \, \right\rangle_\phi \circ Z^{-1} \right), \tag{60}$$

where we use (D.9).

The eigenvalues of $\hat{H}$ are the same as the eigenvalues of $\hat{M}$, which are given by $f \circ I$ evaluated at $I = (n + 1/2)\hbar$, or as we shall prefer to write it, $f \circ A$ evaluated at $A = (n + 1/2)\hbar$ (in this final step we are starting to confuse the functions I, A, with the values I, A). We compose $f \circ I = f_0 \circ I + \hbar^2 f_2 \circ I + \dots$ with Z and use (37), (48) and (60) to obtain (1), which is the Bohr-Sommerfeld formula including $O(\hbar^2)$ corrections.

Equation (1) is manifestly invariant under linear canonical transformations, since the matrix $J^{\mu\nu}$ is invariant under conjugation by a symplectic matrix. Therefore, although this equation was derived in coordinates (x, p) with balanced units of action$^{1/2}$, the original units may be restored by a canonical scaling transformation, and the answer remains the same.

In the case $H = p^2/2m + V(x)$, we have $\{H, H\}_2 = 2V''(x)/m$, and (1) agrees with the second order results of Bender and Orszag (1978), although we omit the details of the comparison. Equation (1) also agrees with the recent result of Colin de Verdière (2004). We have also derived (1) by a completely different method (a kind of WKB-Maslov method), and obtained the same answer. We believe (1) is correct.

5.2. Action operators

The formalism presented naturally suggests a definition of an "action operator." Let $\hat{V}$ be the overall unitary transformation resulting from the composition of the preparatory and second stage transformations,

$$\hat{V} = \dots \hat{U}_4 \hat{U}_2 \hat{U}, \tag{61}$$

so that

$$\hat{M} = \hat{V} \hat{H} \hat{V}^\dagger = f(\hat{I}). \tag{62}$$

We then define an action operator $\hat{B}$ by

$$\hat{B} = \hat{V}^\dagger \hat{I} \hat{V}, \tag{63}$$

so that

$$\hat{H} = \hat{V}^\dagger f(\hat{I}) \hat{V} = f(\hat{B}). \tag{64}$$

This is the relation whose expression in terms of symbols is the Bohr-Sommerfeld formula. It is straightforward to write out the symbol B of $\hat{B}$ in a power series in $\hbar$. Our analysis of the multidimensional Bohr-Sommerfeld formula involves action operators in a more intimate way than the one-dimensional case.

One can also transform creation and annihilation operators. Let $\hat{a} = (\hat{x} + i\hat{p})/(\sqrt{2}\hbar)$, $\hat{a}^\dagger = (\hat{x} - i\hat{p})/(\sqrt{2}\hbar)$, so that $\hat{I} = (\hat{a}^\dagger \hat{a} + 1/2)\hbar$, and define the unitarily equivalent operators $\hat{b} = \hat{V}^\dagger \hat{a} \hat{V}$, $\hat{b}^\dagger = \hat{V}^\dagger \hat{a}^\dagger \hat{V}$. In this way many of the algebraic relations involving creation and annihilation operators for the harmonic oscillator go over to more general oscillators, for example, $\hat{B} = (b^\dagger b + 1/2)\hbar$.

6. Conclusions

We conclude by presenting some comments on the present calculation.

We could have expanded H in a power series in $\hbar$, as in (5), and used the boundary conditions $H_{n\epsilon} = H_n$ at $\epsilon = 1$, which would have made all the symbols of this paper, $H_{n\epsilon}$, K_n, M_n, etc., independent of $\hbar$. We did not do this because the odd powers of $\hbar$ in the expansion of H would complicate all subsequent formulas without otherwise raising any new, essential issues to be dealt with. The essence of the procedure we have given is one that operates only with even powers of $\hbar$.

In the calculation above there was a "miraculous" cancellation of the K_0-term (58), where in one instance it arose as a consequence of doing the ϵ-integral for K_2, and in the second as a consequence of working out the symbol of a function of an operator. One suspects that this cannot be accidental. We will provide a deeper insight into this cancellation in our subsequent work on the multidimensional problem.

The derivation of the multidimensional generalization of the Bohr-Sommerfeld formula (including order $\hbar^2$ corrections), also known as the Einstein-Brillouin-Keller or torus quantization rule, requires new diagrammatic methods not considered in this paper. The answer is not an obvious generalization of the one-dimensional formula, and it involves some new geometrical issues for its interpretation. These topics will be the subject of a companion paper.

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Appendix A. Notation for Moyal star product

The Moyal star product $A * B$ of two symbols A, B is the symbol of the operator product $\hat{A}\hat{B}$. We write the $\hbar$ expansion of this product in the following notation,

$$A * B = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i\hbar}{2}\right)^n \{A, B\}_n. \tag{A.1}$$

We call the bracket $\{\ ,\ \}_n$ that occurs in this series the "n-th order Moyal bracket" (other authors use this terminology to mean something else). This bracket is defined as follows. First, we define the Poisson tensor and its inverse by means of component matrices in the $z^\mu = (x, p)$ coordinates,

$$J^{\mu\nu} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \qquad J_{\mu\nu} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{A.2}$$

Note that $J_{\mu\nu}$ are the components of the symplectic form. We use $J^{\mu\nu}$ or $J_{\mu\nu}$ to raise and lower indices. This proceeds much as in metrical geometry, but one should note the sign change in

$$X^\mu Y_\mu = -X_\mu Y^\mu. \tag{A.3}$$

(In this paper we sum over repeated indices.) Next, we define

$$\{A, B\}_0 = AB, \tag{A.4a}$$

$$\{A, B\}_1 = A_{,\,\mu}\, J^{\mu\alpha}\, B_{,\,\alpha}, \tag{A.4b}$$

$$\{A, B\}_2 = A_{,\,\mu\nu}\, J^{\mu\alpha} J^{\nu\beta}\, B_{,\,\alpha\beta}, \tag{A.4c}$$

$$\{A, B\}_3 = A_{,\,\mu\nu\sigma}\, J^{\mu\alpha} J^{\nu\beta} J^{\sigma\gamma}\, B_{,\,\alpha\beta\gamma}, \tag{A.4d}$$

etc., as required for (A.1) to be the standard Moyal series for the star product. Note that $\{\ ,\ \}_1$ is the usual Poisson bracket. In this paper a bracket $\{\ ,\ \}$ without a subscript will be assumed to be a Poisson bracket. Note also that

$$\{A, B\}_n = (-1)^n \{B, A\}_n. \tag{A.5}$$

Finally, note that if $\hat{C} = [\hat{A}, \hat{B}]$, then the Moyal series for the symbol of the commutator is

$$\begin{aligned} C = [A, B]_* &= 2 \sum_{n=1,3,5,\ldots} \frac{1}{n!} \left(\frac{i\hbar}{2}\right)^n \{A, B\}_n \\ &= i\hbar \left(\{A, B\} - \frac{\hbar^2}{24} \{A, B\}_3 + \frac{\hbar^4}{1920} \{A, B\}_5 - \ldots \right), \end{aligned} \tag{A.6}$$

which defines the notation $[A, B]_*$.

In this paper we make use of an alternative, diagrammatic notation for n-th order Moyal brackets and related expressions. For example, the ordinary Poisson bracket is be written

$$\{A, B\} = \ A \rightarrow B\ , \tag{A.7}$$

where the arrow indicates differentiations applied to the operands A and B, connected by the $J^{\mu\nu}$ tensor. The base of the arrow is attached to the first index of $J^{\mu\nu}$ and the tip to the second index. The operands can be placed in any position, as long as the arrow goes in the right direction:

$$A \rightarrow B \ = \ \begin{matrix} A \\ \downarrow \\ B \end{matrix} \ = \ \begin{matrix} B \\ \uparrow \\ A \end{matrix} \ = \ B \leftarrow A\ . \tag{A.8}$$

But if the direction of the arrow is reversed, then there is a sign change, due to the antisymmetry of $J^{\mu\nu}$:

$$A \twoheadrightarrow B \;= -\,(A \twoheadleftarrow B)\;, \tag{A.9}$$

which is the usual antisymmetry of the Poisson bracket. Similarly, the second Moyal bracket is given by

$$\{A,B\}_2 = \; A \rightrightarrows B \;=\; A \leftrightarrows B\;. \tag{A.10}$$

The two expressions on the right are equal because changing the direction of both arrows changes the sign twice. In this notation, the Jacobi identity is

$$[\,(A \twoheadrightarrow B) \twoheadrightarrow C\,]+[\,(B \twoheadrightarrow C) \twoheadrightarrow A\,]+[\,(C \twoheadrightarrow A) \twoheadrightarrow B\,] = 0, \tag{A.11}$$

where the square brackets are only for clarity. The first term can be expanded out by the chain rule, which in diagrammatic notation gives

$$(A \twoheadrightarrow B) \twoheadrightarrow C \;=\; (A \twoheadrightarrow B \twoheadrightarrow C) \;+\; (C \twoheadleftarrow A \twoheadrightarrow B)\;. \tag{A.12}$$

Similarly expanding the other two terms gives the vanishing sum of six diagrams, providing a diagrammatic proof of the Jacobi identity.

Appendix B. Notation for functions

In this paper it is convenient to use the (slightly nonstandard) notation $f : A \to B$ to mean that the domain of function f is some suitably chosen subset of set A (in the standard notation, A itself is the domain).

For the calculations of this paper it is important to avoid the usual abuse of notation in physics in which a function is confused with the value of a function. (Actually it is practically impossible to avoid this everywhere, but we shall do so wherever it is likely to cause confusion.) A "function" means a mapping, for example, $H, H_\epsilon, G_\epsilon, \ldots : \mathbb{R}^2 \to \mathbb{R}$, and a canonical transformation is another mapping, $Z_\epsilon, Z, \ldots : \mathbb{R}^2 \to \mathbb{R}^2$. The components $\mu = 1, 2$ of Z or Z_ϵ will be denoted Z^μ or Z^μ_ϵ; each of these is a function : $\mathbb{R}^2 \to \mathbb{R}$. Functions will be denoted by bare symbols, H, Z^μ, etc., whereas values of functions will involve the specification of an argument, $H(z)$, $Z^\mu(z_0)$, etc. It is also important to distinguish the identity map $\mathrm{Id} : \mathbb{R}^2 \to \mathbb{R}^2$ from its value, which are the coordinates themselves. The identity map is defined by

$$\mathrm{Id}^\mu(z) = z^\mu. \tag{B.1}$$

One must also be careful about notation for derivatives. We use comma notation for derivatives since notation such as $\partial A/\partial z^\mu$ prejudices the choice of symbol to be used for the argument of the function. For example, the notation

$$\frac{\partial A}{\partial z^\mu}\big(Z(z)\big) \tag{B.2}$$

is ambiguous; do we differentiate first and then substitute $Z(z)$ for the argument, or substitute first and then differentiate? To avoid this problem, we write $A_{,\mu}$ for the derivative of A, $A_{,\mu} \circ Z$ if we wish to differentiate first and then substitute, and $(A \circ Z)_{,\mu}$ if we wish to substitute first and then differentiate, where $\circ$ represents the composition of two functions. The latter expression can be expanded by the chain rule,

$$(A \circ Z)_{,\,\mu} = (A_{,\,\nu} \circ Z) Z^\nu_{,\,\mu}. \tag{B.3}$$

Poisson and Moyal brackets defined in (A.4*a*)–(A.4*d*) always denote functions. For example, the notation $\{A(z), B(z)\}$ is meaningless, because it is only possible to take the Poisson bracket of functions, not numbers (the values of functions). On the other hand, $\{A, B\}(z)$ is meaningful.

Appendix C. The smoothness of Z

The Moyal product rule (A.1) involves derivatives of symbols, and is not meaningful as it stands if the symbols are not smooth. We are assuming that H is smooth, but there is the question of the smoothness of the transformation Z as we have constructed it. We believe that under the our assumptions about H, the transformation Z is smooth, over a domain which is the open interior of a level set of H surrounding the fixed point but lying inside the first separatrix. We have not proved this, but in the following we present some considerations relevant to the question. We also present an example in which some of our assumptions about H are violated and Z is not smooth.

There are two canonical transformations that are used in the construction of Z, one taking us from $z = (x, p)$ to (ϕ, A), and the other from $z = (x, p)$ to (θ, I). The transformation Z defined by (37) is the composition of one of these canonical transformations with the inverse of the other. These two canonical transformations are smooth except where θ or ϕ jumps from 0 to 2π, and except at the fixed point, where $I = A = 0$ and θ or ϕ is undefined. Therefore Z is also smooth, except possibly at these places.

Let the transformation from $z = (x, p)$ to (θ, I) be given by

$$\begin{aligned} x &= \sqrt{2I}\sin\theta, \\ p &= \sqrt{2I}\cos\theta, \end{aligned} \tag{C.1}$$

which amounts to a convention for the origin of the angle θ (it lies along the p-axis). This transformation is written without regard to the warnings of Appendix B, but if we think of $z^\mu = (x, p)$ as values ($\in \mathbb{R}$) and θ and I as functions, then the equation is put into proper notation by writing the left hand side as $\mathrm{Id}^\mu(z)$ and θ and I on the right hand side as $\theta(z)$ and $I(z)$. Thus, (C.1) expresses the relation between the functions Id^μ and functions (θ, I). Now composing this with Z gives

$$Z^\mu = \begin{pmatrix} \sqrt{2A}\sin\phi \\ \sqrt{2A}\cos\phi \end{pmatrix} \tag{C.2}$$

which gives an explicit representation of functions Z^μ in terms of functions A and ϕ. In particular, this shows that Z is continuous when ϕ jumps from 0 to 2π, as long as $A \neq 0$.

The inverse transformation can be handled in a similar way. Let the transformation from $z^\mu = (x, p)$ to (ϕ, A) be expanded in a Fourier series in ϕ,

$$z^\mu = \sum_n z_n^\mu(A)\, e^{in\phi}, \tag{C.3}$$

where $z_n^\mu : \mathbb{R} \to \mathbb{C}$ are the expansion coefficients. This is subject to the same warnings about abuse of notation as (C.1). When these are straightened out and the result is composed with Z^{-1}, we obtain

$$(Z^{-1})^\mu = \sum_n (z_n^\mu \circ I)\, e^{in\theta}, \tag{C.4}$$

an explicit representation of Z^{-1}.

Now we wish to show that Z is smooth at the fixed point. This means that Z has derivatives of all orders. In the following we present algorithms which we believe correctly give the derivatives of Z and of other functions at the fixed point, although we do not attempt to prove this in detail.

Since H is smooth, it has an expansion about the fixed point,

$$H(z) = \frac{1}{2} Q_{\mu\nu}\, z^\mu z^\nu + \dots, \tag{C.5}$$

where for simplicity we assume that the fixed point is at $z = 0$ and that the constant term in the expansion vanishes, and where $Q_{\mu\nu}$ is the positive definite Hessian matrix (6) evaluated at the fixed point. This series need not converge, but all coefficients in the series (the derivatives of H) are defined. It is convenient to manipulate such power series in a formal manner, since the rules for manipulating power series (multiplying, inverting, composing, etc.) are equivalent to the rules (chain, Leibnitz, etc.) for expressing the derivatives of new functions in terms of given derivatives of old ones.

Birkhoff normal form theory (Birkhoff, 1927; Dragt and Finn, 1976; Eckhardt, 1986) is a convenient way of developing a power series expansion of the transformation Z. This theory takes a Hamiltonian represented as a power series in $z = (x, p)$, whose leading term is a harmonic oscillator, and transforms it into a function of the harmonic oscillator action I. The expansion (C.5) of H does not begin with a harmonic oscillator, but can be brought into this form by means of a linear canonical transformation $L : \mathbb{R}^2 \to \mathbb{R}^2$, as shown by the theory of normal forms for quadratic Hamiltonians (Arnold, 1989). That is, there exists linear symplectic map L such that

$$(H \circ L)(z) = \frac{1}{2} a_1 (x^2 + p^2) + \dots, \tag{C.6}$$

where $a_1 > 0$, and where the ellipsis represents cubic and higher terms in a power series. In this step we rely on the positive definiteness of $Q_{\mu\nu}$. Then Birkhoff normal form theory provides another (nonlinear) canonical transformation $N : \mathbb{R}^2 \to \mathbb{R}^2$, represented as a power series in z in which the leading (linear) term is the identity transformation, such that $H \circ L \circ N$ is a function of I,

$$H \circ L \circ N = f_0 \circ I = a_1 I + a_2 I^2 + \dots, \tag{C.7}$$

where f_0 is the same function introduced in (34) and (35). The coefficients a_1, a_2, etc. are determined by Birkhoff normal form theory, and they give the derivatives of function f_0, which is smooth at the fixed point. We remark that in a one-dimensional problem such as this one, there are no resonance conditions so the Birkhoff algorithm can be carried to any order in the power series.

It follows from (C.7) and (35) that $A = I \circ Y$, where $Y = (L \circ N)^{-1}$, so Y has the same effect on I as does Z in (37). This does not mean that $Y = Z$, because Y does not necessarily satisfy the second of equations (37). But $\theta \circ Y$ is an angle variable conjugate to A, so it differs from ϕ only by some phase shift δ that depends on A. Assuming this phase shift is well behaved at $A = 0$ (this is really an assumption of reasonableness on the definition of ϕ), there exists another canonical transformation S smooth at $z = 0$ so that $Z = Y \circ S$ satisfies both halves of (37). In this way all the derivatives of Z at $z = 0$ may be computed.

We note that if our conditions on H are not met, then Z need not be smooth at the fixed point. For example, the relation between action and energy for the quartic oscillator ($V(x) = x^4$) is given by $H = cA^{4/3}$, so $K_0 = H \circ Z^{-1} = c'(x^2 + p^2)^{4/3}$,

where c and c' are constants. Thus, K_0 is not smooth at the fixed point, and neither is Z.

Appendix D. Notation for averaging operators

This appendix develops abuse-free notation for the averaging operator introduced in subsection 4.1. Let $Q : \mathbb{R}^2 \to \mathbb{R}$ be a function on phase space, treated as a Hamiltonian with evolution parameter α,

$$\frac{dz^\mu}{d\alpha} = J^{\mu\nu} Q_{,\,\nu}(z), \tag{D.1}$$

where we assume Q is independent of α so the equations are autonomous (unlike the case of G_ϵ considered above). Let $Y_\alpha^Q : \mathbb{R}^2 \to \mathbb{R}^2$ be the associated flow, with components $(Y_\alpha^Q)^\mu$. The superscript Q indicates the Hamiltonian function generating the flow. The flow functions satisfy

$$\frac{d(Y_\alpha^Q)^\mu}{d\alpha} = J^{\mu\nu}(Q_{,\,\nu} \circ Y_\alpha^Q) = \{(Y_\alpha^Q)^\mu, Q\}. \tag{D.2}$$

We will be interested in the case that Q is an action variable, I, A_ϵ, or A.

For example, with $Q = I$, we have an advance map Y_α^I that advances the angle θ by α. That is, if a point z of phase space has action-angle coordinates (θ, I), then the point $Y_\alpha^I(z)$ has coordinates $(\theta + \alpha, I)$. Thus averaging over the angle θ can be written as

$$\bar{F} = \int_0^{2\pi} \frac{d\alpha}{2\pi} F \circ Y_\alpha^I = \langle F \rangle_\theta, \tag{D.3}$$

which defines the notation $\langle F \rangle_\theta$. Similarly, we define $\langle F \rangle_{\phi_\epsilon}$ and $\langle F \rangle_\phi$, using the advance maps $Y_\alpha^{A_\epsilon}$ and Y_α^A.

The advance maps Z_ϵ and Y_α are related by the following identity:

$$Z_\epsilon \circ Y_\alpha^{A_\epsilon} = Y_\alpha^I \circ Z_\epsilon. \tag{D.4}$$

In other words, angle evolution and ϵ-evolution commute. We prove this by regarding both sides as functions of α at fixed ϵ, and writing X_α and X'_α for the left and right hand sides, respectively. Note that $X_\alpha = X'_\alpha$ at $\alpha = 0$. The left hand side satisfies the differential equation,

$$\begin{aligned} \frac{dX_\alpha}{d\alpha} &= (Z_{\epsilon,\nu} \circ Y_\alpha^{A_\epsilon}) \frac{d(Y_\alpha^{A_\epsilon})^\nu}{d\alpha} = (Z_{\epsilon,\nu} \circ Y_\alpha^{A_\epsilon}) \{(Y_\alpha^{A_\epsilon})^\nu, A_\epsilon\} \\ &= \{Z_\epsilon \circ Y_\alpha^{A_\epsilon}, A_\epsilon\} = \{X_\alpha, A_\epsilon\}, \end{aligned} \tag{D.5}$$

where we have used the chain rule property of the Poisson bracket. The right hand side satisfies

$$\frac{dX'_\alpha}{d\alpha} = \frac{dY_\alpha^I}{d\alpha} \circ Z_\epsilon = \{Y_\alpha^I, I\} \circ Z_\epsilon = \{X'_\alpha, A_\epsilon\}, \tag{D.6}$$

where we have used (23) and (39*a*). Since X_α and X'_α satisfy the same differential equation and the same initial conditions, they are equal, $X_\alpha = X'_\alpha$, and the identity (D.4) is proven. It can also be written in the form,

$$Y_\alpha^{A_\epsilon} \circ Z_\epsilon^{-1} = Z_\epsilon^{-1} \circ Y_\alpha^I. \tag{D.7}$$

It follows from this that for any function F on phase space,

$$\left\langle F \circ Z_\epsilon^{-1} \right\rangle_\theta = \langle F \rangle_{\phi_\epsilon} \circ Z_\epsilon^{-1}. \tag{D.8}$$

In view of (39*b*) this is a plausible identity. In particular, at $\epsilon = 1$ we have

$$\left\langle F \circ Z^{-1} \right\rangle_\theta = \langle F \rangle_\phi \circ Z^{-1}. \tag{D.9}$$

To prove (D.8), we express the left hand side as an integral, and then apply (D.7):

$$\int_0^{2\pi} \frac{d\alpha}{2\pi}\, F \circ Z_\epsilon^{-1} \circ Y_\alpha^I = \int_0^{2\pi} \frac{d\alpha}{2\pi}\, F \circ Y_\alpha^{A_\epsilon} \circ Z_\epsilon^{-1}. \tag{D.10}$$

Appendix E. Function G_ϵ exists

Let Z_ϵ^μ be an ϵ-dependent canonical transformation, defined on a contractible region. We wish to show that there exists a function G_ϵ such that (19) is satisfied. Write $S^\mu{}_\nu = Z^\mu_{\epsilon,\nu}$ for the derivatives of Z_ϵ, which form a symplectic matrix. Then

$$\frac{dZ_\epsilon^\mu}{d\epsilon} = S^\mu{}_\alpha J^{\alpha\beta} G_{\epsilon,\beta}, \tag{E.1}$$

or

$$G_{\epsilon,\beta} = J_{\beta\alpha}(S^{-1})^\alpha{}_\mu \frac{dZ_\epsilon^\mu}{d\epsilon} = S^\alpha{}_\beta J_{\alpha\mu} \frac{dZ_\epsilon^\mu}{d\epsilon} \tag{E.2}$$

where we use the property of symplectic matrices, $S^t J S = J$, where J is the matrix with components $J_{\mu\nu}$. We must show that the second derivatives $G_{\epsilon,\beta\gamma}$ are symmetric. Differentiating, we find

$$G_{\epsilon,\beta\gamma} = S^\alpha{}_{\beta,\gamma} J_{\alpha\mu} \frac{dZ_\epsilon^\mu}{d\epsilon} + S^\alpha{}_\beta J_{\alpha\mu} \frac{dS^\mu{}_\gamma}{d\epsilon}. \tag{E.3}$$

The first term on the right hand side is symmetric in (β, γ), since

$$S^\alpha{}_{\beta,\gamma} = Z^\alpha_{\epsilon,\beta\gamma}, \tag{E.4}$$

and the second term is also, as we see by differentiating $S^t J S = J$ with respect to ϵ and juggling indices. Thus, the function G_ϵ exists.

Appendix F. A transformation of the integrand of (52)

In this Appendix to save writing we drop the ϵ subscripts on $H_{0\epsilon}$, G_ϵ, A_ϵ and ϕ_ϵ, writing simply H_0, G, A and ϕ. The latter symbols, however, are not to be confused with the notation indicated in Table 1 at $\epsilon = 1$. We have placed this part of the calculation in an Appendix, to avoid confusion due to the notational change.

Let us pick out the ϕ-average of the Moyal bracket in the integrand of (52) and write it in an obvious notation,

$$\left\langle\, G \rightleftarrows H_0 \,\right\rangle_\phi = \int_0^{2\pi} \frac{d\phi}{2\pi}\ (G \rightleftarrows H_0)\ , \tag{F.1}$$

where the parentheses are only for clarity. We now introduce a technique for "breaking a bond" of an angle-averaged graph that is sometimes useful. The average of course depends only on A, if we think of it as a function of (ϕ, A). We imagine evaluating this average at constant action $A = a$, which we enforce by inserting a δ-function and integrating over both A and ϕ. This transforms (F.1) into

$$\int \frac{dA\, d\phi}{2\pi}\, \delta(A - a)\ (G \rightleftarrows H_0)\ , \tag{F.2}$$

where the integral is taken over a region of phase space that includes the level set $A = a$ (an orbit of H_0). We then transform variables of integration to $z = (x, p)$, we

use $dA\,d\phi = d^2z$ (since the transformation is canonical), we write out one of the bonds explicitly, and we integrate by parts in the variable z^ν:

$$\int \frac{d^2z}{2\pi}\,\delta(A-a)\;(G_{,\,\mu} \rightrightarrows H_{0,\nu})\;J^{\mu\nu} = -\int \frac{d^2z}{2\pi}\Big[\delta'(A-a)\,A_{,\,\nu}\;(G_{,\,\mu} \rightrightarrows H_0) + \delta(A-a)\;(G_{,\,\mu\nu} \rightrightarrows H_0)\Big]J^{\mu\nu}. \tag{F.3}$$

The second term in the final integral vanishes, due to the symmetry of $G_{,\,\mu\nu}$ and the antisymmetry of $J^{\mu\nu}$. In the first term we switch variables of integration back to (ϕ, A) and do the A-integration, which gives

$$\int \frac{d\phi}{2\pi}\,\frac{\partial}{\partial A}\;(A \leftarrow G \rightrightarrows H_0) \;= -\frac{d}{dA}\left(\frac{1}{\omega\circ A}\left\langle\; H_0 \rightarrow G \rightrightarrows H_0 \;\right\rangle_\phi\right), \tag{F.4}$$

where we use $H_0 = f_0 \circ A$, that is, (40), and $\omega = f_0'$, and change the direction of an arrow in the final form.

Appendix G. An antiderivative for the integral (53)

In this Appendix we use the same notational simplifications as in Appendix F.

In guessing an antiderivative that will allow us to do the integral (53), we must express the diagram $H_0 \rightarrow G \rightrightarrows H_0$, which contains one G and three arrows, as $D/D\epsilon$ of some other diagram. We note by (25) that taking $D/D\epsilon$ of a diagram introduces both G and an extra arrow. Therefore taking the antiderivative must remove G and one arrow. The only diagram we can form from two copies of H_0 and two arrows is $H_0 \rightrightarrows H_0$, so we compute,

$$\frac{1}{2}\frac{D}{D\epsilon}\;(H_0 \rightrightarrows H_0) \;= \left(\frac{dH_0}{d\epsilon} \;\rightrightarrows H_0\right) - \frac{1}{2}\;(H_0 \rightrightarrows H_0) \rightarrow G\;. \tag{G.1}$$

The first term can be written,

$$(H_0 \rightarrow G) \rightrightarrows H_0 \;=\; (H_0 \leftleftarrows H_0 \rightarrow G) \;+ 2\left(\begin{array}{c} H_0 \\ \nearrow\;\nwarrow \\ H_0 \rightarrow G \end{array}\right) + \;(H_0 \rightarrow G \rightrightarrows H_0)\;, \tag{G.2}$$

where we use $(16a)$ and the chain rule, while in the second term of (G.1) removing the parentheses provides a factor of 2, thereby cancelling the first term on the right hand side of (G.2). As for the triangle diagram, it vanishes, as we note by writing,

$$\left(\begin{array}{c} G \\ \nearrow\;\searrow \\ H_0 \rightarrow H_0 \end{array}\right) = \left(\begin{array}{c} G \\ \swarrow\;\nwarrow \\ H_0 \leftarrow H_0 \end{array}\right) = -\left(\begin{array}{c} G \\ \nearrow\;\searrow \\ H_0 \rightarrow H_0 \end{array}\right), \tag{G.3}$$

where in the first step we reflect about the vertical line and in the second reverse the directions of all three arrows. The overall result is (54).

Appendix H. The uniqueness of the intermediate Hamiltonian K

In this appendix we study how the intermediate Hamiltonian K changes when the path Z_ϵ through the space of canonical transformations is varied. To do this we compose Z_ϵ with a near-identity, ϵ-dependent canonical transformation that becomes

the identity at $\epsilon = 0, 1$. This is equivalent to replacing Z^μ_ϵ with $Z^\mu_\epsilon + \delta Z^\mu_\epsilon$, where $\delta Z^\mu_\epsilon = \{Z^\mu_\epsilon, F_\epsilon\}$, where F_ϵ is a small, ϵ-dependent function such that $F_\epsilon = 0$ at $\epsilon = 0, 1$. The corresponding variation in the inverse function $(Z^{-1}_\epsilon)^\mu$ can be found by varying $Z^{-1}_\epsilon \circ Z_\epsilon = \mathrm{Id}$, which gives

$$\delta(Z^{-1}_\epsilon)^\mu = -J^{\mu\nu}\, F_{\epsilon,\nu} \circ Z^{-1}_\epsilon. \tag{H.1}$$

Then we vary (28) to obtain,

$$\delta H_{0\epsilon} = \{H_{0\epsilon}, F_\epsilon\}. \tag{H.2}$$

Finally, to get δG_ϵ, we vary (19) to obtain,

$$\frac{d}{d\epsilon}(\delta Z^\mu_\epsilon) = \{\delta Z^\mu_\epsilon, G_\epsilon\} + \{Z^\mu_\epsilon, \delta G_\epsilon\}. \tag{H.3}$$

The first term on the right hand side is $\{\{Z^\mu_\epsilon, F_\epsilon\}, G_\epsilon\}$, while the left hand side is

$$\frac{d}{d\epsilon}\{Z^\mu_\epsilon, F_\epsilon\} = \{\{Z^\mu_\epsilon, G_\epsilon\}, F_\epsilon\} + \left\{Z^\mu_\epsilon, \frac{dF_\epsilon}{d\epsilon}\right\}. \tag{H.4}$$

Rearranging this and using the Jacobi identity gives

$$\left\{Z^\mu_\epsilon, \delta G_\epsilon - \frac{DF_\epsilon}{D\epsilon}\right\} = 0, \tag{H.5}$$

where we use (25), or,

$$\delta G_\epsilon = \frac{DF_\epsilon}{D\epsilon}, \tag{H.6}$$

where we drop a possible ϵ-dependent constant.

In the next few steps we adopt the same notational simplification mentioned at the beginning of Appendix F, and in addition we drop the ϵ subscript on F_ϵ and Z_ϵ. Then we combine (32), (H.1), (H.2) and (H.6) to obtain,

$$\delta K_2 = -\frac{1}{24}\int_0^1 d\epsilon \Bigg[\left\{\frac{dF}{d\epsilon}, H_0\right\}_3 - \{\{F, G\}, H_0\}_3 + \{G, \{H_0, F\}\}_3 - \{\{G, H_0\}_3, F\}\Bigg] \circ Z^{-1}. \tag{H.7}$$

In this integral we perform an integration by parts, specified by

$$\begin{aligned}\frac{D}{D\epsilon}\{F, H_0\}_3 &= \left\{\frac{dF}{d\epsilon}, H_0\right\}_3 + \{F, \{H_0, G\}\}_3 - \{\{F, H_0\}_3, G\} \\ &= \left[\frac{d}{d\epsilon}\left(\{F, H_0\}_3 \circ Z^{-1}\right)\right] \circ Z,\end{aligned} \tag{H.8}$$

which allows us to replace the first term of (H.7) with an exact ϵ-derivative plus two more terms. The exact derivative can be integrated, giving zero because of the boundary conditions on F. What remains is

$$\delta K_2 = -\frac{1}{24}\int_0^1 d\epsilon \Big[-\{F, \{H_0, G\}\}_3 + \{\{F, H_0\}_3, G\} - \{\{F, G\}, H_0\}_3 + \{G, \{H_0, F\}\}_3 - \{\{G, H_0\}_3, F\}\Big] \circ Z^{-1}. \tag{H.9}$$

We now use an identity related to the Jacobi identity for operators, itself a consequence of the associativity of operator multiplication. Let $\hat{A}$, $\hat{B}$ and $\hat{C}$ be any

three operators, and write out the Jacobi identity $[\hat{A},[\hat{B},\hat{C}]]+\text{cyclic}=0$ in symbol form, expanding star commutators according to (A.6). The leading order term is the Jacobi identity for the Poisson bracket, and the next correction term is

$$\{A,\{B,C\}_3\}+\{A,\{B,C\}\}_3+\text{cyclic}=0. \tag{H.10}$$

Using this in (H.9) allows us to write the integrand as

$$\begin{aligned}\{H_0,\{G,F\}_3\}\circ Z^{-1} &= [(\omega\circ A)\{A,\{G,F\}_3\}]\circ Z^{-1}\\ &= -(\omega\circ I)\frac{\partial}{\partial\theta}\left(\{G,F\}_3\circ Z^{-1}\right),\end{aligned} \tag{H.11}$$

where we have expanded the Poisson bracket with H_0 in action-angle variables. Finally, on restoring the ϵ's we have

$$\delta K_2=\frac{1}{24}(\omega\circ I)\frac{\partial}{\partial\theta}\int_0^1 d\epsilon\{G_\epsilon,F_\epsilon\}_3\circ Z_\epsilon^{-1}. \tag{H.12}$$

The variation in K_2 is an exact θ-derivative, as claimed, and M_2 is invariant under variations in the path Z_ϵ.

We do not know whether the space of symplectomorphisms we are considering is simply connected, but if not there arises the possibility of distinct paths Z_ϵ that are not homotopic. Since M_2 is unique, it must be that the difference in K_2 along such paths is still an exact θ-derivative.

Appendix I. Functions of operators vs. functions of symbols

In this appendix we calculate the symbol of a function of an operator, in terms of the symbol of that operator, as a power series in $\hbar$. We briefly describe a Green's function approach to this problem, which as far as we know was first presented by Voros (1977) and which is discussed further by Colin de Verdière (2004). In this appendix we adopt a general notation, in which $\hat{A}$ is any Hermitian operator, f is any function : $\mathbb{R}\to\mathbb{R}$, and $\hat{B}=f(\hat{A})$. The problem will be to find the symbol B in terms of the symbol A.

Let $a\in\mathbb{C}$ and let $\hat{G}_a=1/(a-\hat{A})$ be the Green's operator associated with $\hat{A}$. The symbol G_a of $\hat{G}_a$ may be computed by demanding $G_a*(a-A)=(a-A)*G_a=1$, expanding $G_a=G_{a0}+\hbar G_{a1}+\hbar^2G_{a2}+\ldots$, expanding the Moyal star product, and collecting things by orders in $\hbar$. One finds that only even powers of $\hbar$ occur in the expansion of G_a, and that otherwise it is easy to solve for the leading terms. Through second order, the results are

$$G_{a0}=\frac{1}{a-A}, \tag{I.1a}$$

$$\begin{aligned}G_{a2} &= -\frac{1}{8}\frac{1}{a-A}\left\{\frac{1}{a-A},A\right\}_2\\ &= -\frac{1}{8}\left[\frac{(A\rightrightarrows A)}{(a-A)^3}+2\frac{(A\to A\leftarrow A)}{(a-A)^4}\right].\end{aligned} \tag{I.1b}$$

This is a special case of the symbol of a function of an operator. For the general case, write $\hat{B}=f(\hat{A})$ in the form,

$$\hat{B}=\int_\Gamma\frac{da}{2\pi i}\frac{f(a)}{a-\hat{A}}, \tag{I.2}$$

where the contour Γ runs from $-\infty$ to $+\infty$ just below the real axis, and then returns just above it. On taking symbols of both sides, this becomes

$$B = \int_\Gamma \frac{da}{2\pi i} f(a) G_a, \tag{I.3}$$

or, on substituting the expansion for G_a and doing the integrals,

$$B = f(A) - \hbar^2 \left[\frac{f''(A)}{16} \; (A \rightrightarrows A) \; + \frac{f'''(A)}{24} \; (A \rightarrow A \leftarrow A) \right] + O(\hbar^4). \tag{I.4}$$

The Green's function method becomes tedious at higher orders, but recently Gracia-Saz (2004) has found convenient methods for calculating the higher order terms, including the multidimensional case. It turns out that the fourth order term in (I.4) contains 13 diagrams. The Green's function derivation of (I.4) has required f to be analytic in a strip around the real axis, but Gracia-Saz has shown that the same expansion holds more generally.

It was stated above that an operator is a function of $\hat{I}$ if and only if the symbol is a function of I. We prove this by noting that an operator is a function of $\hat{I}$ if and only if it commutes with the unitary operator $\hat{U}(t) = \exp(-it\hat{I}/\hbar)$ for all t. This follows since the spectrum of $\hat{I}$ is nondegenerate. But the unitary operator $\hat{U}(t)$ is a metaplectic operator (Littlejohn, 1986), so when we conjugate an operator, $\hat{A} \mapsto \hat{U}(t)\hat{A}\hat{U}^\dagger(t)$, the symbol A is rotated in phase space. Therefore an operator commutes with all $\hat{U}$ if and only if its symbol is rotationally invariant in phase space, that is, is a function of I.

The same thing can be proven at the level of $\hbar$ expansions. The general term of the series (I.4) involves diagrams composed of copies of A connected by arrows. But if $A = I$, then all diagrams with three or more arrows attached to any I vanish, since I is a quadratic function of z. Therefore the only nonvanishing diagrams are linear ones and circular ones. A linear diagram with n I's (two on the ends and $n-2$ in the middle) vanishes if n is even, and is $2(-1)^{(n-1)/2} I$ if n is odd. A circular diagram with n I's vanishes if n is odd, and is $2(-1)^{n/2}$ if n is even. Equation (57) is a special case of these rules. For now the point is that both these diagrams are functions of I. Thus the entire series (I.4) is a function of I, for any function f.

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